$HgBa_2CaCu_2O_6$ (Hg-1212) Structure: A2BC2DE6_tP12_123_h_c_g_b_gi-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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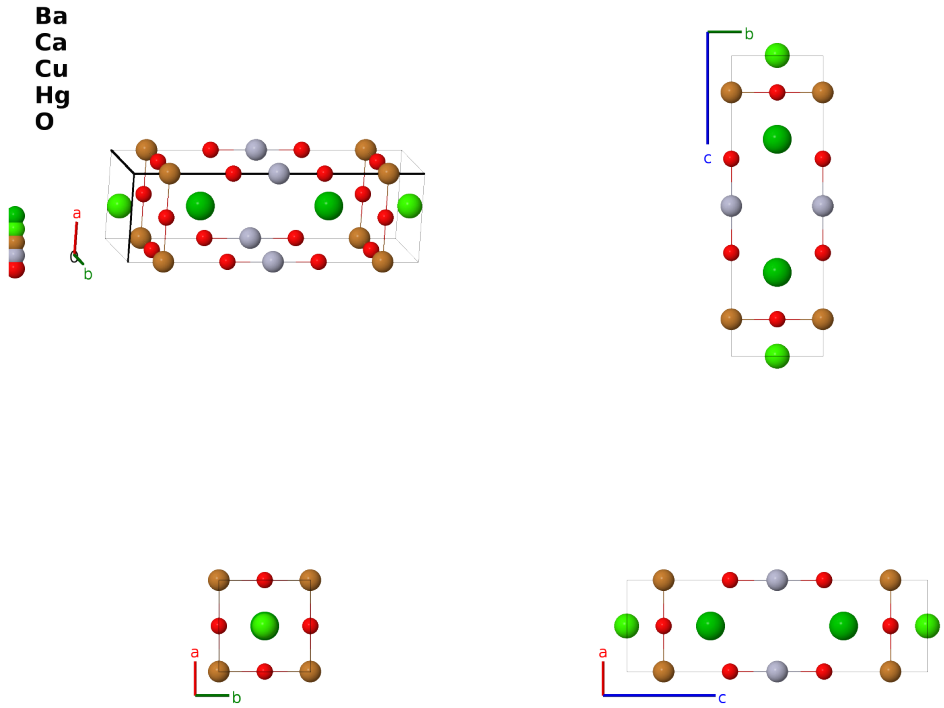
https://aflow.org/prototype-encyclopedia/SY4M

https://aflow.org/prototype-encyclopedia/A2BC2DE6_tP12_123_h_c_g_b_gi-001



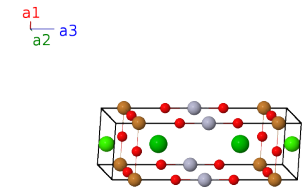
Prototype	$Ba_2CaCu_2HgO_4$
AFLOW prototype label	A2BC2DE6_tP12_123_h_c_g_b_gi-001
ICSD	75725
CCDC	1636369
Pearson symbol	tP12
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=A2BC2DE6_tP12_123_h_c_g_b_gi-001 --params=`$a, c/a, z_3, z_4, z_5, z_6$

Other compounds with this structure
$SnSr_2CaCu_2O_{7-x}$, $TlSr_2PrCu_2O_{7-x}$

- The Hg-12$(n-1)n$, or nHBCCO in the notation of (Bacq-Labreuil, 2025), cuprates have the general formula $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$. These are tetragonally-stacked perovskite-like compounds similar to tetragonal $YBa_2Cu_3O_7 - x$, and all are superconducting at temperatures near or above 100K. Although compounds have been structured for $n \leq 16$ (Bacq-Labreuil, 2025) we will limit ourselves to tabluating the first three. In addition, we will only list the zero-pressure structures and assume perfect stoiciometry. In practice the can be additional oxygen ($\delta > 0$) and a deficit of barium.
- We include the structures
  - Hg1201/1HBCCO: $HgBa_2CuO_4$,
  - Hg1212/2HBCCO: $HgBa_2CaCu_2O_6$ (this structure), and
  - Hg1223/3HBCCO: $HgBa_2Ca_2Cu_3O_8$
- If we replace the calcium atom by copper, this becomes the tetragonal $YBa_2Cu_{3-x}O_{7-y}$ structure. In line with this, excess oxygen in this structure most likely can be found on the (2e) (0 1/2 1/2) site.
- (Hunter, 1994) inadvertently state that their O1 (our O II) site is on Wyckoff position (2e). It is actually at Wyckoff position (4i) as shown here and in the ICSD entry.
- AFLOW shifted the origin of the experimental report of the structure, moving the mercury atom from the (1a) to the (1b) site.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Hg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(1c)	Ca I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2g)	Cu I
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2g)	Cu I
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2g)	O I
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(2g)	O I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2h)	Ba I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(2h)	Ba I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(4i)	O II

$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(4i)	O II

References

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Found in

[1] B. Bacq-Labreuil, B. Lacasse, A.-M. S. Tremblay, D. Sénéchal, and K. Haule, *Towards an* ab initio *theory of high-temperature superconductors: a study of multilayer cuprates*, Phys. Rev. X **15**, 021071 (2025), doi:10.1103/PhysRevX.15.021071.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).